Magnetic susceptibility of hcp iron and the seismic anisotropy of Earth's inner core

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The seismic anisotropy of the Earth's core is believed to be due to a preferred orientation of hexagonal close packed (hcp) iron crystals that constitute the dominating element in the inner core. In this connection, the magnetic properties of the hcp iron in an external magnetic field are very interesting and are studied here by employing an *ab initio* full-potential linear muffin tin orbital method. By this means the magnetic susceptibility χ of hcp iron and its anisotropy energy for pressures and temperatures corresponding to the Earth's inner core conditions have been evaluated in the framework of the local spin density approximation. The accuracy of this method has been validated by calculating the anisotropic susceptibility of paramagnetic transition metals that form in the hcp crystal structure at ambient conditions. Our calculations demonstrate that for hcp iron the anisotropy of χ is dependent on the c/a ratio. In conjunction with recent data on the c/a ratio and elastic constants of hcp iron, the magnetic anisotropy can explain the seismic anisotropy of the Earth's inner core.

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I. INTRODUCTION

Soon after the discovery of seismic anisotropy in the Earth's inner core, which means that elastic waves travel faster in the north-south direction, it was suggested,[1] as an alternative to competing mechanisms,[2–6] that this anisotropy originates from the preferred orientation in an aggregate of structurally and magnetically anisotropic crystals of iron. This mechanism assumes that the magnetic field, generated in the outer core, aligns iron crystals in the inner core, on the condition that these crystals possess a hexagonal close packed crystal structure and an anisotropic magnetic susceptibility χ. Although there is large evidence that the inner core consists of hcp iron, the validity of the proposed magnetic mechanism is substantially dependent on the unknown value of χ of hcp Fe at the inner core, primarily the anisotropy of χ. Also, the assumed anisotropy of the susceptibility of the inner core may have a pronounced effect on the geometry of the geomagnetic field (called the far sided effect[7,8]) and the dynamics of the core.

First principles calculations proved to be a useful tool in modeling of various physical properties of the Earth's core.[3,9–18] Recent *ab initio* total energy calculations for different crystal structures of iron,[3,9,11,13] performed over a wide volume range, as well as recent experimental studies,[19,20] have confirmed the stability of a hcp ground state at high pressures. The hcp phase of iron has also been verified for temperatures and pressures corresponding to the Earth's inner core conditions by employing molecular dynamics simulations[21] and by first-principles pseudopotential calculations of the free energy.[13,17] A substantial progress has also been achieved in theoretical studies of elastic and thermal properties of hcp iron.[11,12,14,17,18] These calculations, however, have not provided a value of χ and its anisotropy for the inner core.

Spin polarized calculations[11,13] have revealed a zero spontaneous magnetic moment for hcp iron at inner core pressures. An antiferromagnetic ground state was proposed for hcp iron by Steinle-Neumann *et al.*,[14] but the relevant pressures appeared to be substantially lower than that of the Earth's inner core. From the experimental side, Mössbauer effect studies[22] have given no confirmation of a magnetically ordered state in hcp iron at pressures up to 24 GPa. A more recent experimental study of magnetic properties of iron, compressed in a diamond anvil cell up to 17 GPa at a temperature of about 260 °C (i.e., far below the Earth's inner core conditions), suggests[23] that hcp iron is either paramagnetic or weakly ferromagnetic with a susceptibility roughly estimated over a very wide range from 10^{-1} to 10^{-4} emu/mol. Also, no information about the anisotropy of χ was available from these experiments. Therefore, there is no way of telling from these studies whether or not the magnetic explanation for the seismic anisotropy is correct.

In order to establish if the magnetic anisotropy explains the seismic anisotropy, one should concentrate on the magnetic properties of hcp iron at pressures and temperatures of the Earth's core. Theoretical works on the magnetic susceptibility of metallic systems have previously been demonstrated to reproduce experiments accurately enough,[24,25] and an avenue to verify the magnetic model for the seismic anisotropy is to study theoretically the susceptibility of hcp iron at the Earth's core conditions, which is the purpose of the present investigation. In this work, we present results of *ab initio* calculations of the magnetic susceptibility of hcp iron over a wide volume range, corresponding to the Earth's inner core conditions.

II. METHOD

Normally only the interaction between the external magnetic field and the electronic spin is considered when one is interested in the magnetic susceptibility of paramagnetic metals. However, the orbital moments in paramagnetic transition metals are by no means negligable, and in fact in many cases they dominate the susceptibility.[24] The calculation of the magnetic susceptibility of metals is a rather difficult problem in solid state physics, which is described in details by Yasui and Shimizu[26] and Benkowitsch and Winter.[27] From a relativistic treatment, based on the Dirac equation, the total susceptibility in the absence of spontaneous magnetic moment can be expressed as the sum[28]

$$\chi_{\mathrm{tot}}=\chi_{\mathrm{P}}+\chi_{\mathrm{so}}+\chi_{\mathrm{orb}}, \tag{1}$$

where χ_{P} is the Pauli spin susceptibility, χ_{orb} is the susceptibility due to the orbital motion of electrons, and χ_{so} corresponds to the contribution due to the spin-orbit coupling. The χ_{so} term is essentially a relativistic correction to the susceptibility,[36,37] and one may assume that it gradually increases from the $3d$ series to the $5d$ and $5f$ series. It has been shown,[28] however, that χ_{so} is a higher order term as compared with χ_{P} and χ_{orb}, and its value was estimated to be much smaller than the other two terms for vanadium.[28,36,37] Hence χ_{so} is usually neglected in theoretical studies of magnetic susceptibility of transition metals.[26,27,29–35] The term χ_{so}, as it was defined by Yasui and Shimizu,[26,28] is not included *explicitly* within the present formalism. On the other hand, we included the effect of the spin-orbit coupling upon the calculated field-induced spin and orbital moments at each variational step in the present calculations, as it was done previously in calculations of χ for $5f$ metals.[24,25]

According to Benkowitsch and Winter,[27] the orbital susceptibility χ_{orb} can be decomposed into three contributions:

$$\chi_{\mathrm{orb}}=\chi_{\mathrm{VV}}+\chi_{\mathrm{dia}}+\chi_{\mathrm{L}}, \tag{2}$$

where these terms correspond to a generalization of the Van Vleck paramagnetism, the Langevin diamagnetism of closed shells, and a generalization of Landau conduction electrons diamagnetism, respectively. In order to evaluate terms in Eqs. (1) and (2), the corresponding wave vector (q) dependent susceptibilities $\chi(q)$ were calculated using a realistic band structure of some transition metals, and then the limit $q\rightarrow 0$ was taken either analytically[27] or by numerical extrapolation.[26,28,36,37] Using a linear response theory, spin and orbital contributions to the magnetic form factor were derived,[29,30] which are related to the corresponding susceptibility terms in the limit of small wave numbers. Another development of linear response formalism based on a Green's functions technique was employed to calculate the spin[32,33,35] and orbital[35] magnetic susceptibilities in a number of transition metals. These calculations were mainly based on a nonmagnetic ground state of transition metals, and the exchange enhancement of the Pauli spin susceptibility was taken into consideration, in the best case, within the Stoner model. More elaborated spin-polarized approaches were proposed by Jarlborg and Freeman[38] and Sandratskii and J. Kübler[39] for the calculation of χ_{P}; however, the orbital contributions to χ_{tot} have not been considered in these works.

In the present paper we propose an alternative approach, which has been shown to have a high reliability in calculating the magnetic susceptibility of metals,[24,25] as described below, even the anisotropic properties of the susceptibility, and is hence an alternative to extracting experimental data for the susceptibility of iron at conditions of the Earth's core. Our calculations are performed using a full-potential linear muffin-tin orbital (FPLMTO)[42] method within the local spin density approximation for exchange-correlation effects, and the Kohn-Sham equations are solved for a general potential without any shape approximation. It should be pointed out, that this implementation of the FPLMTO method has successfully provided elastic constants of hcp transition metals at ambient[43] and elevated pressures,[11] and proved to be reliable in describing bulk properties at high pressure.[44] The volume and crystal structure are the only inputs to calculations of this kind. The details of the method employed are given elsewhere,[11,24,25,42,43] and here we touch only upon principal features of the present implementation, which are different from other used FPLMTO techniques. The integration over the k space was performed using a special point sampling of about 2000 k points in the irreducible part of the Brillouin zone. We also have taken into account the Fermi-Dirac distribution corresponding to a number of temperatures up to the estimated Earth's inner core temperature of 6000 K. In the present calculations the basis set included the ns and np orbitals as well as the $(n+1)s$, $(n+1)p$, and nd orbitals within a single, fully hybridizing, energy panel,[42] where n is the principal quantum number for a corresponding transition metal.

All relativistic effects, including spin-orbit coupling, were included at each variational step in the present calculations. Under the Earth's inner core pressure the conduction electrons are pushed closer to the nuclei with a consequent increase of the kinetic energy. Therefore, the relativistic effects can be of considerable significance even for comparatively "light" elements, like Fe. The effect of an external magnetic field **B** was taken into account self-consistently by means of the Zeeman operator:

$$H_{\mathrm{Z}}=\mathbf{B}\cdot(2\mathbf{s}+\mathbf{l}), \tag{3}$$

where **s** is the spin operator and **l** the orbital angular momentum operator. This operator was incorporated in the FPLMTO Hamiltonian for *ab initio* calculations of field-induced spin and orbital magnetic moments, in an analogous way to spontaneously spin-polarized systems.[45] It has been shown previously[24,25] that including the full Zeeman operator is essential in order to calculate the magnetic susceptibility of d and f metals. The orbital polarization correction,[46] corresponding to Hund's second rule, was also taken into account in the calculations. For iron one can hardly expect an appreciable effect of this correction on χ_{orb}, unlike in the actinides.[24,25,46] Nevertheless, it seems important to include all relativistic effects on the same footing to provide a sufficient accuracy for calculations of the anisotropy of χ_{orb}.

When the field induced spin and orbital magnetic moments are calculated, the corresponding volume magnetization can be evaluated, and the ratio between the magnetization and the field strength provides a susceptibility, which corresponds to the sum of the χ_{P}, χ_{so}, and χ_{VV} terms in Eqs. (1) and (2), derived in the framework of different calculation techniques.[28,35,36] The components of the magnetic susceptibility, $\chi_{\parallel}$ and $\chi_{\perp}$, were derived from the magnetic moments obtained in an external field, applied parallel and perpendicular to the c axis, respectively. In the present calculations, as well as in previous ones for cubic metals,[24,25] we have tested the induced magnetization in different external magnetic fields, and found it linear in the fields of 0.5–10 T. This proves that the calculated susceptibility is independent on the strength of the field. The number of 2000 k points provides relative precision better than 10% for the calculated $\Delta\chi$, or about $10^{-5}\mu_B$ for corresponding field-induced moments, using an external field of 10 T. For lower fields, like 0.5 T, a huge number of k points (about 100000) appeared to be necessary to get the desirable convergence for $\Delta\chi$. The extra computational efforts are obviously not needed, since $\Delta\chi$ is correctly calculated with a much lower number of k points in a field of 10 T. The corresponding calculated total energies were well converged ($\sim 10^{-6}$ Ry) with respect to all parameters involved, such as k-space sampling and basis set truncation.

In the present work we did not calculate the diamagnetic contributions to the susceptibility coming from core and conduction electrons, which corresponds to the χ_{dia} and χ_{L} terms in Eq. (2). The Langevin contributions χ_{dia} have been calculated by Banhart *et al.*[47] for metals with atomic numbers $Z \leqslant 49$ by using self-consistent charge densities. The calculated χ_{dia} appeared to be between free-atom and free-ionic diamagnetic susceptibilities, and did not reveal any anisotropy. To calculate the Landau diamagnetic contribution χ_{L} is a considerably more difficult problem.[26,27,48–50] The free-electron Landau limit is often used for estimations, giving a χ_{L} that equals $-\frac{1}{3}$ of the Pauli spin susceptibility, though for some systems this crude approximation was found not to provide even the correct order of magnitude of the diamagnetic susceptibility.

III. MAGNETIC SUSCEPTIBILITY

Before discussing the calculated results for hcp iron, we first inspect the accuracy of the present method, by comparing experimental and theoretical data for the susceptibility of paramagnetic hcp transition metals. Although the above mentioned theoretical studies were mainly focused on cubic transition metals,[26–28,35–37] some investigations of magnetic susceptibility of hcp metals were carried out as well, namely by Liu *et al.*[30] (Sc, Y, Zr, Lu), Bakonyi and Ebert[31] (Zr), Matsumoto *et al.*[33] (Sc, Y), and Bakonyi *et al.*[34] (Ti, Zr, Hf). Unfortunately, some important contributions to χ, namely χ_{VV}, have not been calculated in these studies. Also, Liu *et al.*[30] actually obtained the exchange enhancement of the spin susceptibility χ_{P} by fitting to experimental data. Despite these shortcomings, it has been demonstrated qualitatively[30,33] that susceptibilities of Sc, Y, and Lu (i.e., the hcp transition metals) are predominantly determined by the spin contribution χ_{P}, whereas in the group IVA of Ti, Zr, and Hf, the orbital contributions are comparable to χ_{P}. To our knowledge, no theoretical studies were done on the magnetic susceptibility of the group-VIIIA hcp metals, Ru and Os.

As regards the anisotropy of the magnetic susceptibility, $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$, essentially no calculations have been carried out for the hcp transition metals. Only Matsumoto *et al.*[33] calculated the anisotropy of χ_{P} for Sc and Y, and it appeared to be of opposite sign to the experimental $\Delta\chi$,[40,41] presumably due to the prevailing contribution from the anisotropic orbital susceptibility.

TABLE I. The averaged value of the magnetic susceptibility, $\overline{\chi} = (\chi_{\parallel} + 2\chi_{\perp})/3$, and its anisotropy, $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$, of hcp transition metals (in units of 10^{-6} emu/mol). The experimental data (Refs. 40 and 41) and our calculations for Ti, Zr, Hf, Ru, and Os correspond to ambient pressure and $T = 1000$ K. The calculated susceptibility of hcp iron corresponds to $P = 350$ GPa and $T = 1000$ K. The estimations of Mori (Ref. 52) are related to $T = 0$ K.

HCP	$\overline{\chi}$			$\Delta\chi$	
Metal	Theory	Ref. 52	Expt. (Ref. 40)	Theory	Expt. (Refs. 40 and 41)
Ti	237	138	200	8	10
Zr	154	135	140	10	21
Hf	78	76	90	5	18
Fe	168	212	—	–18	—
Ru	191	243	50	–12	–9
Os	131	253	20	–5	–5

The pioneering works of Kubo and Obata[51] and of Mori[52] were based on the tight binding formalism, which included the main contributions to the susceptibility, corresponding to χ_{P} (without exchange enhancement), χ_{so}, and χ_{VV}. The energy bands of paramagnetic hcp Co were used by Mori[52] for all other hcp transition metals within the rigid band approximation, and obviously the calculated contributions to χ can be considered only as crude estimations, moreover $\Delta\chi$ was not evaluated. However, these contributions to χ are basically consistent with what is calculated in the present work, and therefore these results are given in Table I for comparison.

In the present work, the field-induced spin and orbital magnetic moments were calculated for Ti, Zr, Hf, Ru, and Os, which possess the hcp crystal structure at ambient pressure and reside in two different groups of the Periodic Table. The calculations were performed at the experimental lattice parameters of c and a. The thermal effects in χ were taken into account only via the Fermi-Dirac distribution function, corresponding to the electronic temperature of $T = 1000$ K. The averaged value of the calculated susceptibility, $\overline{\chi} = (\chi_{\parallel} + 2\chi_{\perp})/3$, and its anisotropy, $\Delta\chi$, are listed in Table I. The susceptibilities evaluated in the present work were corrected for the Langevin diamagnetic term χ_{dia}, taken from Banhart *et al.*[47] We estimated the values of χ_{dia} for Hf and Os as -49 and -46×10^{-6} emu/mol, respectively, by extrapolation from the Ti and Zr, and also the Fe and Ru data provided by Banhart *et al.*[47]

This means that only the Landau diamagnetic contribution χ_{L} was not obtained in the present work. Beyond the free-electron limit, χ_{L} can be expressed qualitatively[48–50] as inversely proportional to an average effective mass of conduction electrons, m^*. Therefore this contribution appears to be large in some nontransition metals[48] and semimetals[49,50] (graphite, beryllium, bismuth) with small values of m^*. In transition metals χ_{L} is usually assumed to be negligible[29,30,33] in comparison to considerable paramagnetic contributions, due to the predominantly large effective masses m^*. On the other hand, it was shown previously[48–50] that the anomalous diamagnetism can originate from a tiny group of quasi degenerate electronic states with small m^*, situated in the vicinity of the Fermi energy, and this contribution can be many times higher than the free–electron Landau estimation.

As can be seen from Table I, for Ti, Zr, and Hf the calculated values of $\overline{\chi}$ are in good agreement with experimental data, which indicates that χ_{L} is presumably about the same value as χ_{dia} in these metals, at least at $T \simeq 1000$ K. On the other hand, there is a noticeable difference between the calculated and experimental susceptibilities in the case of Ru and Os, which could arise from a substantial diamagnetic contribution χ_{L}. In the case of a complicated multiband structure of hcp transition metals it is not feasible to calculate correctly or even estimate the χ_{L} contribution, which can be responsible for the noted discrepancy with the averaged experimental χ for Ru and Os. Although the diamagnetism of conduction electrons can contribute noticeably to the total anisotropy of hcp metals *at low temperatures*,[48–50] this contribution, $\chi_{\parallel}^{\mathrm{L}} - \chi_{\perp}^{\mathrm{L}}$, was found to decrease rapidly at elevated temperatures.[41,48,50] Therefore one would expect that at temperatures above 1000 K the anisotropy of the susceptibility in the nonmagnetic hcp transition metals is predominantly due to the orbital Van Vleck-like contribution, which is calculated in the present work.

As seen from Table I, the experimental anisotropy of the magnetic susceptibility[40,41] is reproduced for all studied elements, namely, the calculated $\Delta\chi$ is positive in Ti, Zr, and Hf (group IVA), but $\Delta\chi$ is negative in Ru and Os (group VIIIA). The absolute values of the calculated anisotropy are also in agreement with experiment, with allowance made for the observed[40,41] strong temperature dependence of $\Delta\chi$. Although the vibrational effects were not taken into account, our approach allows one to describe $\Delta\chi$ of Ti, Zr, Hf, Ru, and Os up to $T \sim 1000$ K. We emphasize that the sign and order of magnitude of $\Delta\chi$ are always reproduced by the theory, and this is the important information one needs in order to draw conclusions about the seismic anisotropy of the Earth's inner core.[1,4] It should be noted that the arguments of Karato,[1] Galoshina,[40] and Volkenshtein *et al.*,[41] that the sign of the anisotropy of χ in hcp transition metals correlates with the number of d electrons in a free atom, if it is odd or even, does not always hold, specifically for Os and hcp Fe.

We can now examine in detail the theoretical results for hcp iron. The field-induced magnetic moments of hcp iron were calculated for a number of atomic volumes, corresponding to pressures from 20 to 350 GPa where the hcp phase is stable.[10,11,15–18,21] The c/a axial ratio was taken to be equal to 1.59, which minimizes the total energy of hcp iron at Earth's inner core conditions,[11,13,15–17,21] and conforms with the recent experimental data[20]. In contradiction to these studies, it has been proposed[18] that the c/a ratio of hcp iron increases substantially with temperature, reaching a value of about 1.7 at Earth's inner core conditions. In this connection the field-induced moments were also calculated for c/a values complying with the temperature dependence of the c/a ratio suggested by Steinle-Neumann *et al.*[18]

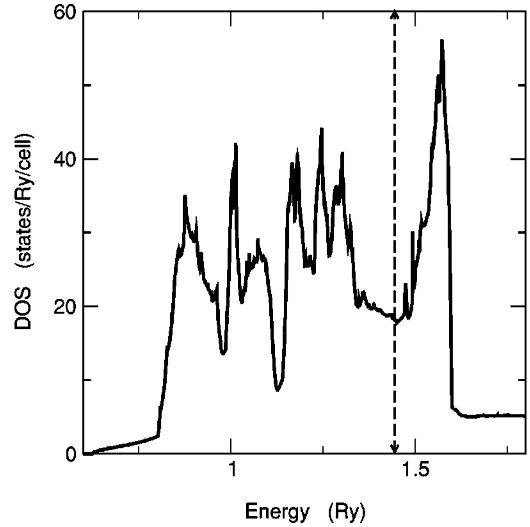

FIG. 1. Density of electronic states of hcp iron at the Earth's core pressure. The Fermi level is marked with a vertical dashed line.

At the conditions of the Earth's core the present theory shows that Fe does not spontaneously order magnetically, and a small magnetic moment develops only in the presence of a magnetic field. This finding is in agreement with results of Söderlind *et al.*[11] and Vočadlo *et al.*,[13] where it was found that under these conditions hcp iron has a vanishing spontaneous magnetic moment. The corresponding density of electronic states (DOS), presented in Fig. 1, is very similar to the DOS of Ru and Os, calculated at ambient conditions.[53]

Our calculations demonstrate that the induced spin moments are parallel to the orbital moments, in agreement with Hund's third rule. The spin contribution to χ appeared to be somewhat smaller than the orbital contribution in hcp Fe ($\chi_{spin} \simeq 0.7\chi_{orb}$ at pressures about 300 GPa), whereas the anisotropy of χ_{spin} ($\sim 10^{-4}$) is substantially smaller than the anisotropy of χ_{orb} ($\sim 10^{-2}$). For comparison, the Pauli spin contribution to the magnetic susceptibility was also calculated within the Stoner model as $\chi_{\mathrm{P}} = 2\mu_{\mathrm{B}}^2 N(1-IN)^{-1}$, where I is the Stoner exchange integral, N the value of the density of states at the Fermi level, and μ_{B} the Bohr magneton. The value of the Pauli susceptibility calculated from this equation is in good agreement with the field induced *spin* susceptibility, evaluated by using the full Zeeman term.

The averaged value of the susceptibility of hcp iron, $\overline{\chi}$, is found to be ranging from 170×10^{-6} emu/mol ($P = 350$ GPa) to 350×10^{-6} emu/mol ($P = 50$ GPa). The corresponding magnetovolume effect, $d \ln \chi / d \ln V$, is presented in Fig. 2, and appeared to be consistent with the available experimental paramagnetostriction data[54] obtained for a few nonmagnetic transition metals.

The calculated susceptibilities $\overline{\chi}$ are consistent with the experimental estimations of χ under lower pressures[23] (P

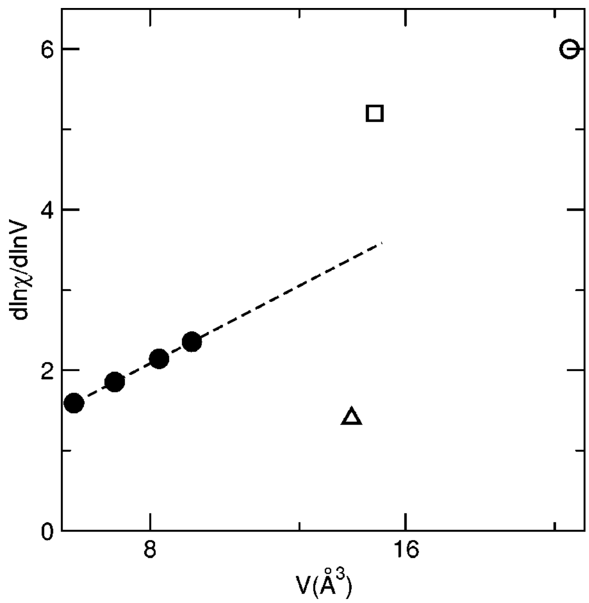

FIG. 2. Calculated magnetovolume effect, $d \ln \chi / d \ln V$, for the hcp iron (in a logarithmic scale). Filled circles represent $d \ln \chi / d \ln V$ at the volume range corresponding to pressures from 350 to 50 GPa, and $T=6000$ K. The dashed line is a guide for the eye. For comparison, the available experimental data (Ref. 54) for $d \ln \chi / d \ln V$ at ambient conditions are presented for vanadium (△), palladium (□), and scandium (○).

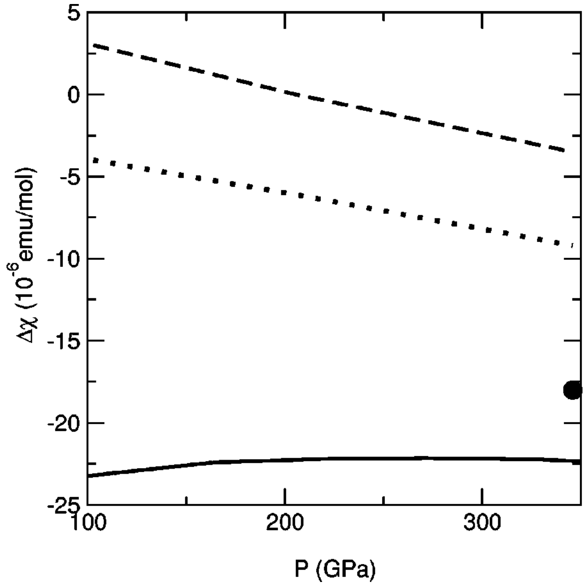

FIG. 3. Pressure dependence of the magnetic susceptibility anisotropy of hcp iron for $c/a = 1.59$. The solid, dotted, and dashed lines correspond to the temperatures 0, 3000, and 6000 K, respectively. The filled circle represents the data from Table I.

$=17$ GPa), and also with the assumptions of Clement and Stixrude,[7] which were actually based upon susceptibilities of Ti, Zr, and Hf at ambient conditions. Table I shows that concerning the anisotropy of χ a comparison of hcp Fe with the group-IVA metals is not justified, since these elements have different signs of $\Delta\chi$ compared to hcp iron. Since Fe is not isoelectronic to Ti, Zr, and Hf, there is no physical reason for why one should expect their magnetic properties to be similar; instead an analogous behavior is actually found for isoelectronic Ru and Os, as is seen in Table I.

IV. SEISMIC ANISOTROPY

We now proceed to the most important finding of this study, namely, the magnetic anisotropy of hcp iron. As can be expected, the anisotropy of χ comes almost exclusively from the orbital contribution. The calculated pressure and temperature dependencies of the magnetic susceptibility anisotropy of hcp Fe are presented in Figs. 3 and 4, respectively.

It has to be emphasized that the atomic volume and the crystal structure were the only inputs to the calculations, which have been done over a wide range of volumes, which well includes the estimated atomic volume of hcp iron in the Earth's core. In order to present the pressure dependence of $\Delta\chi$ in Fig. 3, we preferred to take as input to our calculations volumes corresponding to an equation of state obtained by quasi *ab initio* molecular dynamic (MD) simulations.[21] This choice seems more appropriate for the inner core conditions, but we emphasize that very similar results would have been found by using volumes obtained from a ($T=0$) first principles calculated equation of state. In fact the equation of state calculated in the present work agrees very well with the MD results, and there is a little difference between the MD calculated pressures and our *ab initio* calculated ones. The thermal effects were taken into account through the Fermi-Dirac distribution function, and this approach was successful in describing $\Delta\chi$ of Ti, Zr, Hf, Ru, and Os up to $T \sim 1000$ K, as seen in Table I. This suggests that the lattice vibrations are not expected to change the conclusions about

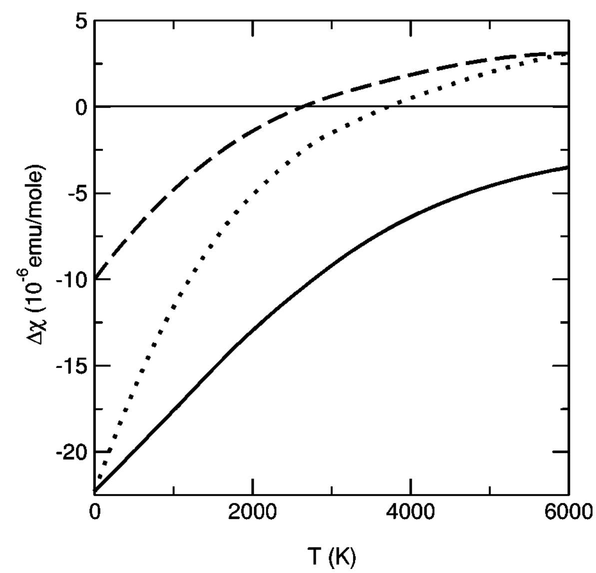

FIG. 4. Temperature dependence of the magnetic susceptibility anisotropy of hcp iron at the Earth's core pressure. The solid and dashed lines correspond to c/a values of 1.59 and 1.7, respectively. The dotted line corresponds to the temperature dependent c/a suggested by Steinle-Neumann *et al.* (Ref. 18).

the magnetic anisotropy. As seen from Figs. 3 and 4, the calculated $\Delta\chi$ and its sign at pressures above 200 GPa dependent on the assumed values of the c/a. That is, at the Earth's core conditions $\Delta\chi$ is negative for c/a proposed to be $\simeq 1.6$,[11,15,16,21] and positive for $c/a \simeq 1.7$, as suggested by Steinle-Neumann *et al.*[18] Such a behavior of $\Delta\chi$ in Fe with respect to c/a is certainly not predictable from simple arguments, but can be deduced from *ab initio* calculations, since the calculated induced moments are determined by a delicate interaction between the Zeeman energy, exchange effects, and spin-orbit coupling. At ambient conditions all hcp transition metals have a c/a ratio close to 1.6, but, as can be seen from Table I, $\Delta\chi > 0$ for Ti, Zr, and Hf, whereas for Ru and Os we find that $\Delta\chi < 0$. This means that the c/a ratio is not the main factor determining the sign of $\Delta\chi$. On the other hand, the suggested value for c/a by Steinle-Neumann *et al.*,[18] at increased temperature and pressure, is huge and this can change the balance between the Zeeman energy, exchange effects and the spin-orbit coupling.

A suggested mechanism of the seismic anisotropy of the Earth's inner core involves the anisotropy of the magnetic susceptibility of hcp iron, and it is argued[1] that if χ is sufficiently anisotropic, a preferential orientation of the hcp crystals may occur. A magnetic field within the inner core can be separated into poloidal and toroidal parts. The toroidal field is considered to be stronger than the poloidal field, and its axisymmetric part encircles the Earth's inner core in the east-west direction,[1,4] providing the possibility for the preferential orientation. The validity of this mechanism is crucially dependent on the elastic anisotropy of hcp iron, which has been shown to be determined by the c/a ratio. That is, with the calculated anisotropy of the elastic constants of hcp Fe for $c/a = 1.59$,[3,12,14] the compressional velocity is faster along the c axis than along the a axis, whereas the reversed situation has recently been put forward for hcp iron with $c/a = 1.7$,[18] i.e., the compressional velocity being faster in the basal plane.

This means that in order to satisfy the magnetic mechanism of seismic anisotropy, $\Delta\chi$ has to be *negative* if $c/a = 1.59$, or *positive* if $c/a = 1.7$. As seen from Fig. 4, these conditions are precisely the ones given by the present calculations. Therefore, in either case of the c/a ratio, the sign of the calculated $\Delta\chi$ is in accordance with the magnetic mechanism of seismic anisotropy,[1,4] provided the elastic anisotropy is correctly evaluated in Refs. 3, 12, 14, and 18, respectively. Hence, irrespective of the exact values of the c/a ratio of hcp Fe at the Earth's core conditions, an issue of uncertainty and recent debate,[17,18] the magnetic anisotropy mechanism is operational.

It should be noted here that the magnitude of the magnetic anisotropy is about ten times smaller than what Karato assumed,[1] and one may argue that the anisotropy is not sufficiently strong to orient the hexagonal iron particles. In order to critically evaluate this assertion we quote the result of Karato, based on energetic grounds, that the criterion for the magnetic effect to be operational is that the ratio (called β) of magnetic anisotropy energy to thermal energy is larger than one, which can be expressed as[1,55]

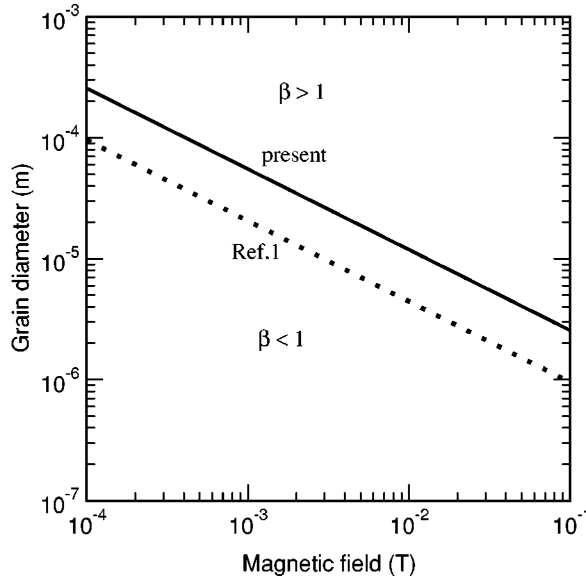

FIG. 5. Phase diagram for the ratio β between magnetic anisotropy energy and thermal energy [Eq. (4)] as a function of the grain diameter and magnetic field. The solid line represents the $\beta = 1$ borderline evaluated in the present work, whereas the corresponding dotted line is taken from Ref. 1.

$$\beta = (1/2)\mu_0 |\Delta\chi| V H^2 / k_B T > 1, \tag{4}$$

where μ_0 is the magnetic permeability of the vacuum, V the volume of iron particles (grains), H the strength of the magnetic field, k_B the Boltzmann constant, and T the temperature. In Fig. 5 we plot a phase diagram, with the diameter of iron grains in the Earth's inner core and the magnetic field of the Earth's core as critical parameters. In the region where β is larger than one the magnetically driven preferential orientation is expected. The results obtained by Karato[1] are also shown in Fig. 5.

An important point is that although the presently calculated value of $\Delta\chi$ is smaller than the value assumed by Karato, this gives little difference in estimated grain size, which is sufficient for the preferential orientation. The reason is that, according to Eq. (4), for a chosen $\beta > 1$ the grain diameter is proportional to $\Delta\chi^{-1/3}$. In the region of interest, i.e., for fields between 10^{-3} and 10^{-2} T, particles with a grain diameter larger than $\sim 5 \times 10^{-5}$ m have enough anisotropy energy for the preferential orientation. It has been suggested that the grains of the Earth's core have diameters substantially larger than this,[1] and our analysis hence shows that, together with the recent data of anisotropy of the elastic constants in hcp iron, the present theoretical calculations of the anisotropy of the magnetic susceptibility demonstrate that the magnetic anisotropy model can explain the seismological experiments.

V. CONCLUSION

We have demonstrated that the seismic anisotropy of the Earth's inner core could have its origin in the anisotropy of the magnetic susceptibility of hcp iron. Our theoretical calculations reproduce the measured anisotropy of many hcp transition metals, and at conditions of the Earth's core they give a sufficient value of $\Delta\chi$ of hcp iron. In addition we show that, depending on the value of the c/a ratio, the anisotropy of the magnetic susceptibility of hcp Fe is either negative or positive. However, since this change in sign is accompanied by a suggested change in elastic anisotropy, we can conclude that irrespective of the value of the c/a ratio [1.59 (Refs. 11, 13, 15–17 and 21) or 1.7 (Ref. 18)] the magnetic anisotropy is a strong candidate for the seismic anisotropy of the Earth's core. We also show that the anisotropy of the magnetic susceptibility is mostly of an orbital origin, which indicates that a relativistic treatment is necessary to explain magnetic properties even of comparatively 'light' elements like Fe.

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